

Frequency

50

0

0 60 120 180

Torsion Angle (°)

Figure 10: Histogram of Torsion Angle ( $^{\circ}$ ) for the 1000 lowest energy conformations. The x-axis represents the Torsion Angle in degrees, ranging from 0 to 180. The y-axis represents the percentage of conformations in each bin, ranging from 0 to 50. The distribution is highly skewed towards 180 degrees, with a peak of approximately 50% in the final bin.

Figure 1: Histogram of Torsion Angle (°) for the C1-C2 bond. The x-axis represents the Torsion Angle in degrees, ranging from 0 to 180. The y-axis represents the percentage of molecules in each bin, ranging from 0 to 50. The distribution is bimodal, with a small peak near 0 degrees and a larger peak near 180 degrees.

Torsion Angle Bin (°)	% in Bin
0 - 10	25
10 - 20	5
20 - 30	2
30 - 40	1
40 - 50	0
50 - 60	2
60 - 70	1
70 - 80	0
80 - 90	0
90 - 100	0
100 - 110	0
110 - 120	0
120 - 130	0
130 - 140	0
140 - 150	2
150 - 160	5
160 - 170	25
170 - 180	30

